

1,3-Naphthalenediol
132-86-5 | DTXSID8059631

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 159 °C

Global applicability domain: Inside

Local applicability domain index: 9.36e-01

Confidence level: 5.98e-01

Nearest Neighbors from the Training Set

[Image not found](#)

1,3-Naphthalenediol

Measured: 124

Predicted: 159

[Image not found](#)

Naphthalene-1,7-diol

Measured: 181

Predicted: 165

[Image not found](#)

Naphthalene-1,6-diol

Measured: 138

Predicted: 162

[Image not found](#)

2,6-Naphthalenediol

Measured: 220

Predicted: 185

[Image not found](#)

2,7-Naphthalenediol

Measured: 193

Predicted: 185